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Use of FOCUS_TOXSWA 4.4.3 software for plant protection products and their metabolites in Dutch risk assessment for aquatic ecosystems

W.H.J. Beltman, C. Vink & A. Poot

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Abstract

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TOXSWA calculates exposure concentrations of plant protection products in water and in sediment and is used in risk assessment studies of aquatic organisms. Replacement of the TOXSWA 1.2 software by the more recent FOCUS_TOXSWA software for use with the NL standard scenarios was investigated. The impact of the replacement on the calculated exposure concentrations of parent compounds and of metabolites was determined. For parent substances the calculated exposure concentrations of the two TOXSWA versions were equivalent. Due to a different way to simulate metabolites, the differences in exposure concentrations calculated by the two versions can be large. For the simulation of metabolite substances two approaches are given to handle situations where the formation fraction is not known.

Key words: TOXSWA, plant protection products, exposure assessment, surface water, registration in the Netherlands

Referaat

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TOXSWA berekent blootstellingsconcentraties van gewasbeschermingsmiddelen in water en in sediment voor de risicobeoordeling van aquatische organismen. Onderzocht is of de TOXSWA 1.2 software kan worden vervangen door de meer recente FOCUS_TOXSWA software om te gebruiken met de NL standaardscenario's. De invloed van vervanging van TOXSWA 1.2 door FOCUS_TOXSWA 4.4.3 op de berekende blootstellingsconcentraties van moederstoffen en van metabolieten is bepaald. De berekende blootstellingsconcentraties voor moederstoffen met de twee TOXSWA-modelversies kwamen overeen. Door het verschil in methodiek van het simuleren van metabolieten kunnen er grote verschillen zijn in de berekende blootstellingsconcentraties voor metabolieten berekend door de twee modelversies. Om metabolieten te simuleren, worden twee methoden gegeven voor gevallen waarin de vormingsfractie van de metaboliet niet bekend is.

Trefwoorden: TOXSWA, gewasbeschermingsmiddel, blootstellingsconcentratie, oppervlaktewater, registratie in Nederland

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Preface

The Dutch ministry of Economic Affairs has commissioned Wageningen Environmental Research (Alterra) to investigate replacement of the TOXSWA 1.2 software by the more recent FOCUS_TOXSWA software for use with the NL standard scenarios. Such a replacement was requested by the Dutch Board for the Authorisation of Plant Protection Products and Biocides (Ctgb). To facilitate the implementation of such a replacement FOCUS_TOXSWA was set up for the Dutch standard scenarios, tested and the tests were documented.

Paulien Adriaanse (Wageningen Environmental Research (Alterra) contributed with suggestions on how to discriminate the two methods to simulate metabolites, which helped to prepare and test FOCUS_TOXSWA, enabling its use for simulating the Dutch standard scenarios.

Wim Beltman

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Summary

TOXSWA calculates exposure concentrations of plant protection products in water and in sediment and is used in risk assessment studies of aquatic organisms. TOXSWA software version 1.2 is currently used in the national registration of plant protection products in the Netherlands. The user interface of TOXSWA 1.2 is complemented with parameterisation of NL standard scenarios (i.e. Dutch ditches representing realistic worst cases for a spring and an autumn scenario), can handle parent substances only, and assumes spray drift entries as the only entry route. The FOCUS_TOXSWA software released in 2015 for use in the EU registration process supports the simulation of metabolite formation, which TOXSWA 1.2 does not, and offers improved functionalities for data management of simulation projects. Therefore replacement of the TOXSWA 1.2 software by the more recent FOCUS_TOXSWA software for use with the NL standard scenarios was investigated.

In order to use the FOCUS software, FOCUS_SWASH, SPIN and FOCUS_TOXSWA need to be installed. Additionally a SWASH/TOXSWA database containing the NL standard scenarios and an Excel file with example substances must be downloaded from the TOXSWA website, and installed. A procedure for performing an assessment with the NL standard scenarios is described.

The impact of replacing TOXSWA 1.2 by FOCUS_TOXSWA 4.4.3 on the calculated exposure concentrations of parents and of metabolites was investigated, using test substances based on realistic substances. Simulations were done with both model versions for the spring and for the autumn scenario, using either a single or multiple applications of six example substances. The calculated values of global maximum concentrations in water and in sediment, and time-weighted average exposure concentrations over 21 days (TWAEC21) in water and in sediment were compared.

For the six parent example substances the calculated exposure concentrations of the two TOXSWA versions did not diverge and differences were less than 2% in all simulations for spring, autumn, single and multiple applications.

In TOXSWA 1.2 metabolites are simulated by mimicking their entry into the water as a spray drift event, which is not realistic. FOCUS_TOXSWA 4.4.3 simulates metabolite formation in a realistic way. Due to this difference in the simulation of metabolites, exposure concentrations calculated by the two versions may differ. If information on the formation fraction of metabolites is not known, options to deal with this are: (1) use a formation fraction of 1, or (2) use the maximal fraction observed in the water-sediment study and mimic the formation of the metabolite as a spray drift event (= approach used with TOXSWA 1.2).

The conclusions of the study are: (1) FOCUS_TOXSWA 4.4.3 software can be used to calculate exposure concentrations for the NL standard scenarios, (2) exposure concentrations for parent substances calculated with FOCUS_TOXSWA 4.4.3 are equivalent to those calculated by TOXSWA 1.2, and (3) exposure concentrations for metabolites calculated by using a formation fraction of 1 can differ appreciably from concentrations calculated by using the maximal fraction observed in the water-sediment study and mimicking the formation of the metabolite as a spray drift event. For the simulation of metabolite substances two approaches are given to handle situations where the formation fraction is not known.

Samenvatting

TOXSWA berekent blootstellingsconcentraties van gewasbeschermingsmiddelen in water en in sediment voor de risicobeoordeling van aquatische organismen. TOXSWA-versie 1.2 wordt momenteel gebruikt voor de nationale registratie van gewasbeschermingsmiddelen in Nederland. Het gebruikersinterface van TOXSWA 1.2 bevat de parameterisatie van de Nederlandse standaard-scenario's (d.w.z. Nederlandse sloten onder 'realistic worst case' omstandigheden in het voorjaar en in het najaar). Het model simuleert alleen de moederstof en gaat uit van spuitdrift als de enige aanvoeroute. De FOCUS_TOXSWA-software beschikbaar gekomen in 2015 voor gebruik in het EU-registratieproces heeft de mogelijkheid om vorming van metabolieten te simuleren, wat TOXSWA 1.2 niet kan, en heeft een veel betere functionaliteit voor beheer van simulatieprojecten. Daarom is onderzocht of de TOXSWA 1.2-software kan worden vervangen door de meer recente FOCUS_TOXSWA-software voor gebruik met de Nederlandse (NL) standaardscenario's.

Om de FOCUS-software te kunnen gebruiken, moeten FOCUS_SWASH, SPIN en FOCUS_TOXSWA worden geïnstalleerd. Daarnaast moeten een SWASH/TOXSWA database met de NL-standaard-scenario's en een Excel-bestand met voorbeeldstoffen worden gedownload van de TOXSWA-website, en geïnstalleerd. Een procedure om een beoordeling met de NL-standaardscenario's uit te voeren, is beschreven.

De invloed van vervanging van TOXSWA 1.2 door FOCUS_TOXSWA 4.4.3 op de berekende blootstellingsconcentraties van moederstoffen en van metabolieten is onderzocht, gebruikmakend van teststoffen gebaseerd op werkelijke stoffen. Met beide modelversies zijn simulaties uitgevoerd voor het voorjaarsscenario en het najaarsscenario, met één toediening en met herhaalde toedieningen, met zes voorbeeldstoffen. De berekende waarden van globale maximumconcentratie in water en in sediment, en tijd-gewogen gemiddelde concentraties over 21 dagen (TWAEC21) in water en in sediment zijn vergeleken.

De berekende blootstellingsconcentraties van de moederstof van de zes voorbeeldstoffen van de twee TOXSWA-versies liepen niet uit elkaar en verschillen waren kleiner dan 2% in alle simulaties voor voorjaar, najaar, enkelvoudige en herhaalde toedieningen.

Met TOXSWA 1.2 worden metabolieten gesimuleerd door een spuitdriftgebeurtenis na te bootsen, wat niet realistisch is. FOCUS_TOXSWA 4.4.3 simuleert metabolietvorming op realistische wijze. Door het verschil in methodiek van het simuleren van metabolieten kunnen de berekende blootstellingsconcentraties mogelijk verschillen tussen beide modelversies. Als de vormingsfractie van de metaboliet niet bekend is, dan zijn er twee opties: (1) gebruik een vormingsfractie van 1, of (2) gebruik de maximale fractie aangetroffen in een water-sedimentstudie en simuleer de metaboliet als een spuitdriftgebeurtenis (= methode gebruikt met TOXSWA 1.2).

De conclusies van de studie zijn: (1) FOCUS_TOXSWA-software kan worden gebruikt om blootstellingsconcentraties te berekenen met de NL-standaardscenario's, (2) blootstellingsconcentraties van moederstoffen berekend met FOCUS_TOXSWA 4.4.3 zijn equivalent aan concentraties berekend met TOXSWA 1.2, en (3) blootstellingsconcentraties van metabolieten berekend door gebruik te maken van een vormingsfractie van 1 verschillen aanzienlijk van concentraties berekend met de maximale fractie aangetroffen in een water-sedimentstudie en simuleren van de metaboliet als een spuitdriftgebeurtenis. Om metabolieten te simuleren, worden twee methoden gegeven voor gevallen waarin de vormingsfractie van de metaboliet niet bekend is.

1 Introduction

1.1 Background

TOXSWA calculates exposure concentrations of plant protection products in water and in sediment and is used in risk assessment studies of aquatic organisms. TOXSWA version 1.2 is currently used in the national registration of plant protection products in the Netherlands. The user interface of TOXSWA 1.2 is complemented with parameterisation of standard scenarios i.e. Dutch ditches representing realistic worst cases, and assumes spray drift entries of parent substances as the only entry route (Beltman and Adriaanse, 1999a; Beltman and Adriaanse, 1999b). In this report we refer to these standard scenarios used for the calculation of exposure concentrations in water and sediment of ditches as 'the NL standard scenarios'.

Replacement of TOXSWA 1.2 by a more recent version of the model, FOCUS_TOXSWA version 4.4.3 released in 2015 was explored. FOCUS_TOXSWA 4.4.3 is subsequently also called FOCUS_TOXSWA 4, where "4" indicates that it is the fourth of specific FOCUS versions released. The two main reasons for the exploration to replace version 1.2 by version 4 are:

1. FOCUS_TOXSWA 4.4.3 supports the simulation of metabolite formation, which TOXSWA 1.2 does not.
2. The data management of simulation projects is poorly supported in TOXSWA 1.2, and version 4 offers much better functionalities. The users of TOXSWA benefit from an instrument which offers better possibilities to organize, manage and archive simulation projects.

Therefore the current study investigates whether FOCUS_TOXSWA 4.4.3 can replace TOXSWA 1.2 as the new instrument for simulation of the fate of plant protection products and their metabolites for the NL standard scenarios.

The FOCUS_TOXSWA 4.4.3 software can be used as available from the FOCUS website, but also needs a replacement database that contains the scenario parameters of the NL standard scenarios.

Metabolites are currently calculated with TOXSWA 1.2 by mimicking their entry into the water as spray drift event, which is not realistic. FOCUS_TOXSWA 4.4.3 simulates metabolite formation in a more realistic way, but this may result in large differences in the calculated exposure concentrations of the metabolites between the two TOXSWA versions. These differences are the consequence of the improvement of metabolite assessment. In this report two options are presented for dealing with the different way of simulating metabolites with FOCUS_TOXSWA 4.4.3: (1) use a formation fraction of 1, or (2) use the maximal fraction observed in the water-sediment study and mimic the metabolite as a spray drift event (which is equivalent to the approach used with TOXSWA 1.2).

1.2 Objectives and approach

The objectives of this report/study are:

1. To describe the use of the FOCUS_TOXSWA 4.4.3 software for calculation of exposure concentrations for the NL standard scenarios.
2. To investigate the impact of replacing TOXSWA 1.2 by FOCUS_TOXSWA 4.4.3 on calculated exposure concentrations of parents and of metabolites; verification that the exposure concentrations of parent substances calculated by the two TOXSWA versions are similar. The research questions are:
 - (a) for parents; do both versions of TOXSWA give the same exposure concentrations, and
 - (b) for metabolites; how large are the differences in exposure concentrations between the two versions.

To address objective 1, we devised a procedure for using the FOCUS_TOXSWA 4.4.3 software such that simulations of NL standard scenarios can be performed. We prepared input of FOCUS_TOXSWA 4.4.3 for the NL standard scenarios, using the parameterisation of these scenarios given in TOXSWA 1.2. An important requirement for the procedure developed to use FOCUS_TOXSWA 4.4.3 for simulating exposure concentrations of the NL standard scenarios is user friendliness. The procedure for using FOCUS_TOXSWA 4.4.3 for simulating exposure concentrations of the NL standard scenarios is described in Chapter 2.

To address research question (2a) we tested whether calculations using kernels of FOCUS_TOXSWA 4.4.3 and of TOXSWA 1.2 resulted in similar exposure concentrations for parent compounds.

Test substances based on realistic substances were defined. Simulations were performed using both model versions. The exposure concentrations that were compared are the global maximum concentration in water and in sediment, and time weighted average exposure concentration over 21 days (TWAEC21) in water and in sediment. If the parameterisation for FOCUS_TOXSWA 4.4.3 and the different TOXSWA kernel versions resulted in comparable (i.e. differing by less than 2%) results, the use of FOCUS_TOXSWA was considered acceptable. The simulations and results are described in Chapter 3.

To address research question (2b) we (i) describe for both model versions how metabolite exposure concentrations are simulated, (ii) indicate the difference between the two methods and (iii) describe how these differences affect the exposure concentrations; some illustrative graphs of concentrations as function of time are given for both model versions. Methods for simulating metabolite exposure, differences between the methods and impact of these differences on the simulated exposure concentrations of metabolites are described in Chapter 4.

1.3 Short description of the NL standard scenarios

Two scenarios were defined to calculate exposure concentrations from spray drift inputs (Beltman and Adriaanse, 1999a); a spring scenario and an autumn scenario. The spring scenario is representative for spring and summer. The scenarios represent a ditch of 320 m long, bottom width of 0.4 m, and a slope of 1:1. The water layer is 0.30 m deep, contains 15 mg/L suspended solids with 50% organic matter and contains no macrophytes. The sediment layer contains 25% organic matter in the top segment decreasing with depth to 2% in the deepest segment ending at 0.1 m depth. The flow velocity and water depth in the two scenarios are constant in time, and along the ditch. The only difference between the two scenarios is the flow velocity; in the spring scenario it is 10 m/d (dispersion coefficients 20 m²/d) and in the autumn scenario it is 100 m/d (dispersion coefficients 200 m²/d). Parent substances enter the water layer via spray drift in the stretch from 20 to 320 m. TOXSWA calculates exposure concentrations in water and in sediment for these scenarios.

1.4 TOXSWA 1.2

TOXSWA version 1.2 simulates the fate of plant protection products in waterbodies with constant flow (Adriaanse, 1996; Beltman and Adriaanse, 1999b). TOXSWA 1.2 was developed in 1997 – 1999 at SC-DLO, predecessor of Wageningen Environmental Research (Alterra). Exposure concentrations in water and in sediment are simulated and can be used for the risk assessment of aquatic organisms. TOXSWA 1.2 is used in the Dutch risk assessment of aquatic organisms by simulating spray drift entries of parent substances in the spring and autumn scenarios described in section 1.3. TOXSWA 1.2 does not support simulation of the formation of metabolites. At present, the fate of metabolites are simulated indicatively by mimicking their formation as a spray drift event. The method used is described in Chapter 4. The kernel TOXSWA version 1.2 is embedded in a Graphical User Interface (version 1.0). The software does not comprise a database. Input and output files of the simulation runs are stored in folders on the computer. An example of the main screen of the GUI is shown in Figure 1.

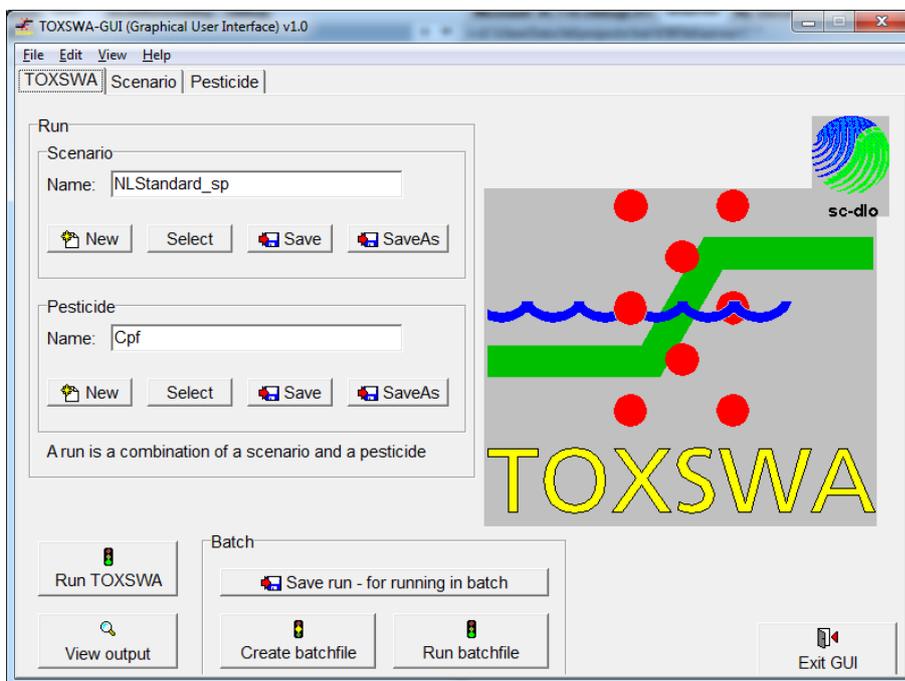


Figure 1 Main screen of TOXSWA GUI v1.0 embedding TOXSWA kernel v1.2.

1.5 FOCUS_TOXSWA 4.4.3

FOCUS_TOXSWA simulates the fate of plant protection products in systems with either constant or variable flow. FOCUS_TOXSWA was developed in 1999 – 2002 for use with the EU FOCUS scenarios (FOCUS, 2003). FOCUS_TOXSWA versions 1.1.1, 2.2.1 and 3.3.1 were used for simulation of the fate of parent substances due to entries of spray drift, drainage and runoff into ponds, ditches and streams. The fate of metabolites that are formed in soil and entering the waterbody through drainage or runoff is also simulated.

FOCUS_TOXSWA 4.4.3 simulates the formation of metabolites in water and in sediment (Adriaanse *et al.*, 2014; Beltman *et al.*, 2014). With this version of TOXSWA, exposure concentrations of parents, soil metabolites, water metabolites and sediment metabolites can be calculated for the EU scenarios.

FOCUS_TOXSWA consists of a TOXSWA kernel, a graphical user interface (see Figure 2) and a database. The database stores the scenario parameterisations, and is filled with the inputs of the model simulations. The database of FOCUS_TOXSWA is shared with FOCUS_SWASH and is part of the FOCUS_SWASH software package. FOCUS_SWASH is a tool to set up simulation runs for the FOCUS surface water scenarios used in the EU authorization process. FOCUS_TOXSWA 4.4.3 uses the Substances Plug IN (SPIN). The SPIN database tool stores pesticide properties, which can be accessed by different pesticide models from Wageningen Environmental Research (Alterra), so substances contained within this database can be used in several models.

FOCUS_TOXSWA 4.4.3 has been set up to enable users to enter their own parameterizations for surface water runs, including the use of the constant flow option used in TOXSWA 1.2. Hence FOCUS_TOXSWA 4.4.3 can be used for the NL standard scenarios by supplying a database with the NL standard scenarios. The new functionality to simulate the formation of metabolites in water and in sediment can then be used for the NL standard scenarios. Furthermore, the up-to-date graphical user interface and databases (SWASH and SPIN) provide a more secure and more user-friendly way of setting up simulation runs, analysing the results and storing the simulation runs.

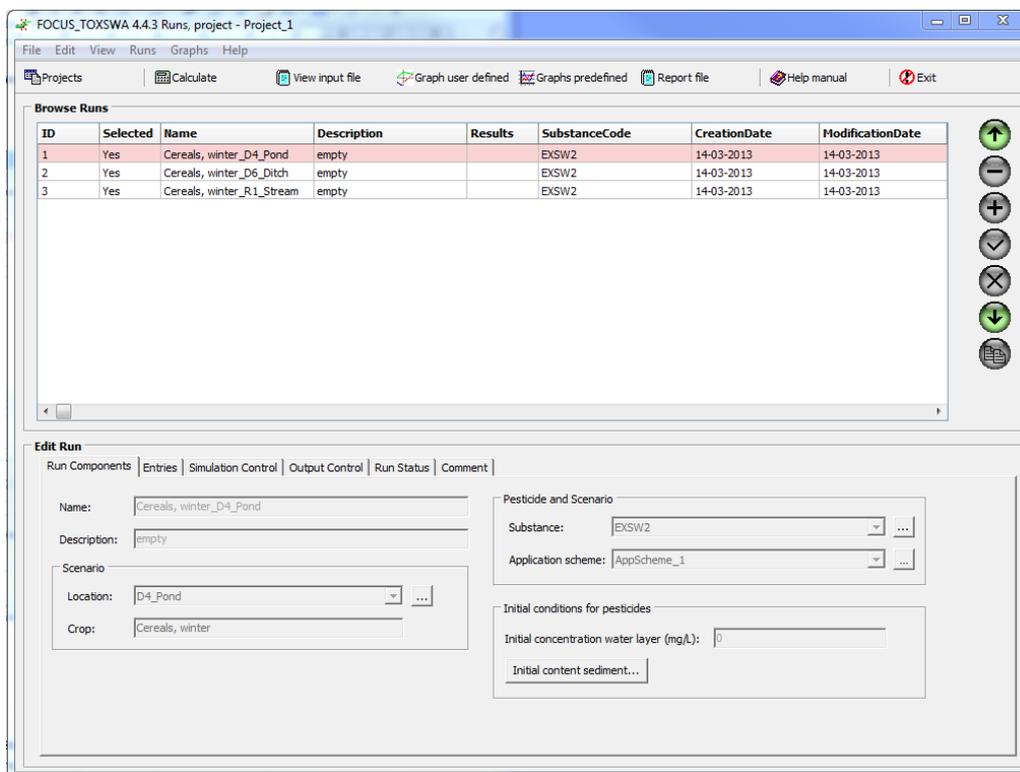


Figure 2 Project form of FOCUS_TOXSWA 4.4.3.

1.6 Report structure

The background and a concise description of the NL standard scenarios and the two models have been presented in Chapter 1. The installation of the software and instructions on how to perform a simulation is described in Chapter 2. The comparison of exposure concentrations of parent compounds calculated by TOXSWA 1.2 and FOCUS_TOXSWA v.4 is described in Chapter 3. Methods for simulating the metabolite exposure, as well as the differences between the two calculation methods and impact of these differences on the simulated exposure concentrations of metabolites are described and illustrated with example calculations in Chapter 4. A short discussion and the conclusions are given in Chapter 5.

2 Installation of software and running TOXSWA

2.1 Installation of software

The software applications needed to run the NL standard scenarios with FOCUS_TOXSWA are: SWASH 5.3, SPIN 2.2 and FOCUS_TOXSWA 4.4.3, or newer versions of these applications, and a SWASH/TOXSWA database containing the NL standard scenarios.

The software applications can be downloaded from the Surface Water pages of the FOCUS website <http://esdac.jrc.ec.europa.eu/projects/focus-dg-sante>. Instructions for installation of an application are given in a readme file that is part of the software package.

When an application has been installed the user manual of the application can be accessed via Help in the menu bar. The manuals of SWASH and TOXSWA can also be downloaded:

- [FOCUS_TOXSWA 4.4.3](#) Beltman *et al.* (2014).
- [SWASH 5.3](#) Van den Berg *et al.* (2015)
- [SPIN 1.1](#) Van Kraalingen *et al.* (2013)

A SWASH/TOXSWA database containing the NL standard scenarios and an Excel file with example substances can be downloaded as a single software package from the TOXSWA website: <http://www.pestidemodels.eu/toxswa/download>.

The SWASH database contains an example project with an example of the two NL standard scenarios: Spring scenario and Autumn scenario.

The Excel file for uploading substance properties into SPIN contains two substances. These are EXNL0; an 'empty' substance which uses default values for many of the parameters, and EXNL1; an example substance, which can be used to do a test run. This example substance was also used in the TOXSWA 1.2 software package.

To finalize the setup go through the following steps:

1. Replacement of the installed SWASH database by the database with NL standard scenarios.
 - Go to the \SWASH\data map.
 - Rename the existing database SWASH.FDB (e.g. to SWASH_FOCUS.FDB).
 - Copy the downloaded database SWASH.FDB that contains the NL standard scenarios to the \SWASH\data map.

The SWASH database containing the FOCUS scenarios has been replaced by a SWASH database containing the NL standard scenarios. When this database is coupled to SWASH, the SWASH application itself cannot be used anymore. However, SWASH is not required for using the NL standard scenarios with TOXSWA.

When SWASH needs to be used for FOCUS again, then rename the database reverse wise (copy SWASH.FDB to e.g. SWASH_NL.FDB, and copy or rename SWASH_FOCUS.FDB to SWASH.FDB).

2. Uploading the substance data into the SPIN database.
 - Start the SPIN application.
 - In the Menu bar, select File, Import
 - Select NL_Substances.csv.

The substances EXNL0 and EXNL1 have been added to the SPIN database. For detailed instructions concerning importing and exporting substances also see the SPIN manual.

3. Performing a test run (not required; for a detailed description see section 2.2)

- Start FOCUS_TOXSWA .
- Select and open project "NL".
- Click Calculate.

The two runs, one for the Spring scenario and one for the Autumn scenario, both use substance EXNL1. The results of the two runs can be viewed in the report file and in the graphs. The exposure concentrations needed for the risk assessment are found at the bottom of the report (and also at the bottom of the sum file). The run with the Spring scenario is the same as the run described in the manual of TOXSWA 1.2 (Beltman and Adriaanse, 1999a). The input file of TOXSWA can be viewed using the View button. Relevant parts of the input file for the NL standard Spring scenario with substance EXNL1 are given in Annex 1. For a detailed description of input and output see the user manual of FOCUS_TOXSWA 4.4.3 (Beltman *et al.*, 2014).

2.2 Execution of a TOXSWA simulation

This section describes how a run with TOXSWA within FOCUS_TOXSWA 4.4.3 can be performed in a simple way, either by copying an example run, or by adding a new run.

The easiest way is to copy and adjust an existing project:

1. In the *Projects* window: copy the example project "NL", and give it a suitable name.
2. Select and open the copied project.
3. Select the *Run components* tab at bottom half of the *Runs, project* window.
4. Click on the button with the icon of 3 dots at the right-hand side of the *Substance* field. The SPIN GUI is started. Add and parameterize a substance. Copy the substance EXNL0 and give it a name. The default parameters have been set. The other parameters have to be entered. After finalizing the substance, exit SPIN.
5. Select a run, or copy a run and select the copied run.
6. Select the substance prepared in the third step from the pulldown menu of the *Substance* field.

Steps 7 to 9 are only required where appropriate.

7. Click on the button with the icon of 3 dots at the right-hand side of the *Application scheme* field. Add an application scheme or edit an existing one. For each application specify the dosage, drift percentage and date of application. Close the *Application schemes and applications* window.
8. Select *Simulation control* tab at bottom half of the *Runs, project* window.
9. Extend the *End date of simulation* to the date of the final application (as specified in the application scheme) + 28 days (to obtain a proper Time Weighed Average Exposure Concentration over 28 days).
10. Top half of the *Runs, project* window: select the runs that should be performed by double-clicking in the corresponding field in the column *Selected*.
11. Click Calculate.
12. View Report file: the exposure concentrations can be read from the file (see lines highlighted in yellow in Figure 3).

It is also possible to make a new run using the + button on the right-hand side of the *Runs, project* window. The following issues should then be addressed in addition to the steps described above for a copy of the run in project "NL":

1. Tab *Simulation Control*: select *Begin date simulation* 1 January 1985 and choose an End date as specified in Step 9 above.
2. Tab *Entries*: All entries, Start and End position: 20 and 320 m
3. Tab *Output control*: Change the *Depth of target layer* into 0.01 m.

* Tables: Maximum exposure concentrations in water layer
 * In segment from 316.00 to 320.00 m in water body
 * Actual concentrations PECsw as well as PECsed refer to momentary concentrations
 * occurring 1, 2 etc days after the global maximum concentration.
 * The Time Weighted Average Exposure Concentrations (TWaec) have been calculated
 * for a moving time frame and have been allocated to the last day of the period considered

* Table: PEC in water layer of substance: EXNL1

| | Concentration µg.L-1 | Date | Daynr |
|------------------------|-------------------------|-------------------|-------|
| Global max | 4.304 | 10-Oct-1985-00h00 | 10 |
| (incl. suspend.solids) | 4.762 | 10-Oct-1985-00h00 | 10) |
| PECsw_1_day | 3.520 | 11-Oct-1985-00h00 | 11 |
| PECsw_2_days | 2.953 | 12-Oct-1985-00h00 | 12 |
| PECsw_4_days | 2.223 | 14-Oct-1985-00h00 | 14 |
| PECsw_7_days | 1.634 | 17-Oct-1985-00h00 | 17 |
| PECsw_14_days | 1.016 | 24-Oct-1985-00h00 | 24 |
| PECsw_21_days | 0.7142 | 31-Oct-1985-00h00 | 31 |
| PECsw_28_days | - | - | - |
| PECsw_42_days | - | - | - |
| PECsw_50_days | - | - | - |
| PECsw_100_days | - | - | - |

* Legend: - in table means PECsw is later than end of simulated period: 30-Oct-1985

* Table: Maximum Time Weighted Averaged Exposure Concentrations substance: EXNL1

| | Concentration µg.L-1 | Date | Daynr |
|------------------|-------------------------|-------------------|-------|
| TWaecsw_1_day | 3.888 | 11-Oct-1985-00h00 | 11 |
| TWaecsw_2_days | 3.554 | 12-Oct-1985-00h00 | 12 |
| TWaecsw_4_days | 3.053 | 14-Oct-1985-00h00 | 14 |
| TWaecsw_7_days | 2.557 | 17-Oct-1985-00h00 | 17 |
| TWaecsw_14_days | 1.917 | 24-Oct-1985-00h00 | 24 |
| TWaecsw_21_days | 1.562 | 31-Oct-1985-00h00 | 31 |
| TWaecsw_28_days | - | - | - |
| TWaecsw_42_days | - | - | - |
| TWaecsw_50_days | - | - | - |
| TWaecsw_100_days | - | - | - |

* Tables: Maximum exposure content in sediment

* In the top 1.00 cm sediment located under
 * the water body segment from 316.00 to 320.00m,
 * the content is expressed as µg substance per kg dry sediment.

* Table: PEC in sediment of substance: EXNL1

| | Content µg.kg-1 | Date | Daynr |
|---------------|--------------------|-------------------|-------|
| Global max | 758.8 | 23-Oct-1985-02h00 | 23 |
| PECsed_1_day | 758.2 | 24-Oct-1985-02h00 | 24 |
| PECsed_2_days | 756.6 | 25-Oct-1985-02h00 | 25 |
| PECsed_4_days | 751.0 | 27-Oct-1985-02h00 | 27 |
| PECsed_7_days | 738.8 | 30-Oct-1985-02h00 | 30 |

Figure 3 Part of the report file of a TOXSWA run with the NL standard spring scenario and substance EXNL1. The lines marked yellow give the exposure concentrations that are relevant for the Dutch risk assessment

3 Comparison of exposure concentrations of parent substances

3.1 Introduction

In this chapter the comparison of the output generated by the two model versions is described for six example substances. The objective of the comparison is to verify that the exposure concentrations of parent substances calculated by the two TOXSWA versions are similar; possible minor differences between the results of the models should be explained. The concentrations in water (peak concentration and Time Weighted Average Exposure Concentration of 21 days, TWAEC21), and the peak concentration in sediment are compared. The TWAEC in sediment generated by the two models is not compared because TOXSWA 1.2 does not provide such a value in the standard output.

The properties of the example substances are chosen in such a way that they cover realistic high and low values.

For each substance simulations were performed for the spring and autumn NL standard scenarios and two different application schemes (i.e. single and multiple applications). In the autumn scenario the flow velocity and dispersion coefficient are a factor 10 larger than in the spring scenario.

3.2 Substance properties and application schemes

The properties of the six example substances are generalized from the properties of existing substances. The substances are thus representative for the wide range of substances submitted for registration. The general characterization of the substances is presented in Table 1. The detailed properties can be found in Table 2. For the Freundlich sorption exponent the default value of 0.9 is used, except for substance 3, where 0.8 is used.

Table 1
General characterization of the six example substances.

| Substance | Characteristics |
|-----------|--------------------------------------|
| 1 | Short DegT50 in water |
| 2 | Short DegT50 in sediment |
| 3 | Long DegT50 in water and in sediment |
| 4 | Volatile ¹ |
| 5 | Low K_{om} |
| 6 | High K_{om} |

Calculations are done for two different application schemes, one consisting of a single application and the other using multiple applications. An overview of the application schemes is given in Table 3. For substances 1 to 4, 1 kg/ha is applied, and for substance 5 and 6, 0.01 kg is applied, assuming 1% spray drift for all applications.

¹ For TOXSWA 1.2 transport coefficients need to be entered to calculate volatilization of the substance from the water layer to the air. For FOCUS_TOXSWA 4 these transport coefficients are calculated in the kernel. The transport coefficients are calculated from the molar mass of the substance. Some users of TOXSWA 1.2 used the transport coefficients that were given for the example substance, chlorpyrifos, as default. Hence, if exposure concentrations were calculated with v1.2 using these values, the exposure concentrations calculated with v4 may differ. This difference will be largest for volatile substances.

Table 2

Properties of the six example substances.

| Substance | Molar mass (g/mol) | Solubility (g/L) | Saturated vapour pressure (Pa) | DegT50 in water at 20 °C (d) | DegT50 in sediment at 20 °C (d) | K _{om} (L/kg) |
|-----------|--------------------|------------------|--------------------------------|------------------------------|---------------------------------|------------------------|
| 1 | 300 | 0.02 | 1.10 ⁻⁵ | 0.2 | 1000 | 600 |
| 2 | 250 | 4 | 7.10 ⁻⁹ | 1000 | 40 | 40 |
| 3 | 400 | 0.02 | 1.10 ⁻⁶ | 1000 | 1000 | 200* |
| 4 | 350 | 0.002 | 0.002 | 75 | 100 | 16 000 |
| 5 | 500 | 10 | 8.10 ⁻¹⁰ | 50 | 1000 | 12 |
| 6 | 450 | 0.00001 | 2.10 ⁻⁷ | 1 | 1000 | 140 000 |

* Freundlich exponent, *N* is 0.8.

Table 3

Application schemes for six example parent substances and using 1% spray drift.

| Substance | Application rate (kg a.i./ha) | Loading spray drift (g/m ²) | Number of applications (-) | Time interval between applications (d) |
|-----------|-------------------------------|-----------------------------------------|----------------------------|----------------------------------------|
| 1 | 1 | 0.001 | 1, 8 | 7 |
| 2 | 1 | 0.001 | 1, 8 | 7 |
| 3 | 1 | 0.001 | 1, 8 | 7 |
| 4 | 1 | 0.001 | 1, 8 | 7 |
| 5 | 0.01 | 0.00001 | 1, 8 | 7 |
| 6 | 0.01 | 0.00001 | 1, 8 | 7 |

3.3 Results and discussion

In this section the exposure concentrations calculated by the two model versions are compared.

Spring scenario, single application

The maximum concentrations of the parent substances after a single application in water and in sediment are given in Table 4. The concentrations calculated in water by the two versions differ less than 0.02%. The concentration in sediment differs less than 0.7% between the two versions. The largest difference in calculated concentration occurs for substances with a low sorption coefficient (i.e. substance 2 and 5). For substance 2 and 5 the calculated concentration in sediment with v4 is 0.57% and 0.66% lower respectively.

Table 4

Peak concentrations of six parent substances in water and in sediment after a single application in spring calculated with v1.2 and with v4.

| Substance | PEC in water v1.2 (µg/L) | PEC in water v4 (µg/L) | Difference (%) | PEC in sediment v1.2 (µg/kg) | PEC in sediment v4 (µg/kg) | Difference (%) |
|-----------|--------------------------|------------------------|----------------|------------------------------|----------------------------|----------------|
| 1 | 4.744 | 4.744 | 0.00 | 50.75 | 50.77 | 0.04 |
| 2 | 4.761 | 4.761 | 0.00 | 66.25 | 65.87 | -0.57 |
| 3 | 4.756 | 4.756 | 0.00 | 147.5 | 147.7 | 0.14 |
| 4 | 4.315 | 4.315 | 0.00 | 795.0 | 795.1 | 0.01 |
| 5 | 0.04761 | 0.04760 | -0.02 | 0.4975 | 0.4942 | -0.66 |
| 6 | 0.01857 | 0.01857 | 0.00 | 2.862 | 2.861 | -0.05 |

In Table 5 the values for TWAEC21 are compared. The largest difference is found for the TWAEC in water of the substance with a low DegT50 in water, substance 1; the TWAEC21 calculated with v4 is 1.18% lower than calculated with v1.2.

Table 5

TWAEC21 of six parent substances in water after a single application in spring calculated with v1.2 and with v4.

| Substance | TWAEC21 in water V1.2 (µg/L) | TWAEC21 in water V4 (µg/L) | Difference (%) |
|-----------|------------------------------------|----------------------------------|-------------------|
| 1 | 0.1438 | 0.1421 | -1.18 |
| 2 | 4.398 | 4.398 | 0.00 |
| 3 | 4.223 | 4.224 | 0.02 |
| 4 | 1.666 | 1.665 | -0.06 |
| 5 | 0.04197 | 0.04200 | 0.07 |
| 6 | 0.00224 | 0.00223 | -0.22 |

Spring scenario, multiple applications

The maximum concentrations in water and in sediment of the parent substances after multiple applications are given in Table 6. The concentrations in water differ by 0.19% or less. The concentrations in sediment differ by 1.05% or less. The largest difference is found for the volatile substance (substance 4). For this substance the calculated concentration in sediment with v4 is 1.05% lower.

Table 6

Peak concentrations of six parent substances in water and in sediment after multiple applications in spring calculated with v1.2 and with v4.

| Substance | PEC in water V1.2 (µg/L) | PEC in water V4 (µg/L) | Difference (%) | PEC in sediment V1.2 (µg/kg) | PEC in sediment V4 (µg/kg) | Difference (%) |
|-----------|--------------------------------|------------------------------|-------------------|---------------------------------------|-------------------------------------|-------------------|
| 1 | 4.748 | 4.748 | 0.00 | 81.50 | 81.68 | 0.22 |
| 2 | 21.89 | 21.86 | -0.14 | 308.8 | 305.8 | -0.96 |
| 3 | 21.57 | 21.56 | -0.05 | 617.5 | 615.9 | -0.26 |
| 4 | 10.01 | 10.01 | 0.00 | 5325.0 | 5323.5 | -0.03 |
| 5 | 0.2054 | 0.2050 | -0.19 | 2.375 | 2.350 | -1.05 |
| 6 | 0.02058 | 0.02058 | 0.00 | 19.88 | 19.87 | -0.03 |

In Table 7 the TWAEC21 in water are compared. The largest difference is found for the substance with a low DegT50 in water, substance 1, where a difference of 5.90% is observed. For the other substances the TWAEC21 differ by 0.32% or less, with lower calculated concentrations for v4.

Table 7

TWAEC21 of six parent substances in water after multiple applications in spring calculated with v1.2 and with v4.

| Substance | TWAEC21 in water V1.2 (µg/L) | TWAEC21 in water V4 (µg/L) | Difference (%) |
|-----------|------------------------------------|----------------------------------|-------------------|
| 1 | 0.4541 | 0.4273 | -5.90 |
| 2 | 19.40 | 19.36 | -0.21 |
| 3 | 19.02 | 19.01 | -0.05 |
| 4 | 7.205 | 7.199 | -0.08 |
| 5 | 0.1803 | 0.1799 | -0.22 |
| 6 | 0.007106 | 0.007083 | -0.32 |

Discussion Spring scenario

For the Spring scenario differences in concentrations calculated by the two versions were less than 2% for all calculated concentrations that were compared, except for the TWAEC21 in water of substance 1 for multiple applications (5.9%). Most concentrations calculated with v4 were lower than the concentrations calculated by v1.2.

Figure 4 shows the concentration of substance 1 in water as a function of time calculated by the two model versions. The concentrations calculated by 1.2 and 4 are the same, as shown in the figure. The difference in calculated TWAEC21 is due to the difference in method for calculation of TWA between the two model versions. TOXSWA v1.2 calculates average values of the concentration for each day. Then for each calculation time step (= 600 s) the TWA is calculated via interpolation of the daily values for the past TWA period. FOCUS_TOXSWA 4.4.3 calculates average values for the concentration for each hour. Then for each hour the TWA is calculated by averaging the hourly values over the past TWA period. Both versions calculate the TWA values for the whole simulation period, and at the end of the simulation select the maximum value.

The v1.2 calculation overestimates the TWA, because it assumes a linear decrease between the daily values, whereas the decrease is exponential (i.e. single first order degradation). The overestimation is highest for substances with short half-lives, reflected by the result for the example substance 1 (DegT50 = 0.2 d), where differences between the calculated TWA21 was 5.9% for the application scheme using multiple applications.

FOCUS_TOXSWA 4.4.3 uses an improved TWA calculation, because it does not assume linear decrease between daily values.

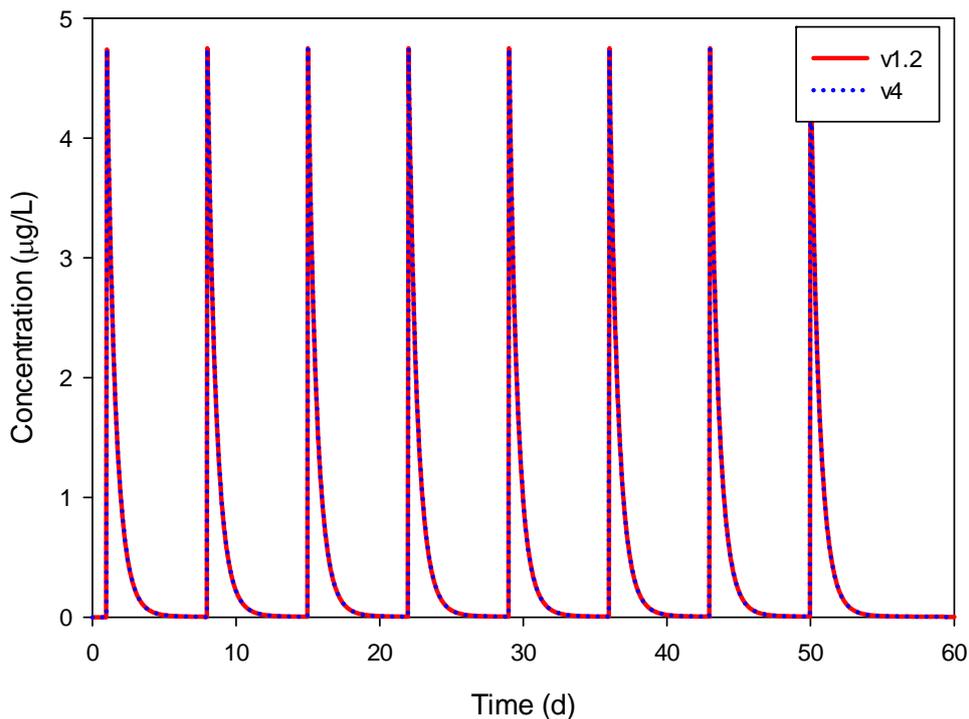


Figure 4 Concentration of substance 1 as a function of time calculated by TOXSWA 1.2 and by FOCUS_TOXSWA 4.4.3. The substance is applied in Spring, 8 times with time interval of 7 d.

Autumn scenario, single application

The results for the Autumn scenarios are given in Table 8. The concentrations calculated in water by the two versions differ less than 0.16%. The concentration in sediment differs less than 0.43% between the two versions. The largest difference in calculated concentration occurs for substances with a low sorption coefficient (i.e. substance 2 and 5). For substance 2 and 5 the calculated concentration in sediment with v4 is 0.42% and 0.43% higher respectively. For all other substances the difference in calculated concentration is less, but higher concentrations are calculated with v4.

Table 8

Peak concentrations of six parent substances in water and in sediment after a single application in autumn calculated with v1.2 and with v4.

| Substance | PEC in water V1.2 (µg/L) | PEC in water V4 (µg/L) | Difference (%) | PEC in sediment V1.2 (µg/kg) | PEC in sediment V4 (µg/kg) | Difference (%) |
|-----------|--------------------------------|------------------------------|-------------------|---------------------------------------|-------------------------------------|-------------------|
| 1 | 4.744 | 4.744 | 0.00 | 50.75 | 50.77 | 0.04 |
| 2 | 4.761 | 4.761 | 0.00 | 52.00 | 52.22 | 0.42 |
| 3 | 4.756 | 4.756 | 0.00 | 100.6 | 100.7 | 0.07 |
| 4 | 4.315 | 4.315 | 0.00 | 505.0 | 505.1 | 0.02 |
| 5 | 0.04761 | 0.04760 | -0.02 | 0.4200 | 0.4218 | 0.43 |
| 6 | 0.01857 | 0.01860 | 0.16 | 2.100 | 2.105 | 0.24 |

In Table 9 the values for TWAEC21 in water are compared. The largest difference is found for the substance with a low DegT50 in water, substance 1; the TWAEC21 calculated with v4 is 1.19% lower than calculated with v1.2. For the other substances the TWA concentrations differ by 0.26% or less, with lower calculated concentrations for v.4.

Table 9

TWAEC21 of six parent substances in water after a single application in autumn calculated with v1.2 and with v4.

| Substance | TWAEC21 in water V1.2 (µg/L) | TWAEC21 in water V4 (µg/L) | Difference (%) |
|-----------|------------------------------------|----------------------------------|-------------------|
| 1 | 0.1423 | 0.1406 | -1.19 |
| 2 | 0.6758 | 0.6743 | -0.22 |
| 3 | 0.6725 | 0.6711 | -0.21 |
| 4 | 0.5366 | 0.5359 | -0.13 |
| 5 | 0.006709 | 0.006700 | -0.13 |
| 6 | 0.001540 | 0.001536 | -0.26 |

Autumn scenario, multiple applications

The maximum concentrations in water and in sediment of the parent substances after multiple applications are given in Table 10. The concentrations in water differ by 0.07% or less. The concentration in sediment differs by 0.90% or less. The largest difference is found for the volatile substance (substance 4). For this substance the calculated concentration in sediment with v4 is 0.90% lower.

Table 10

Peak concentrations of six parent substances in water and in sediment after multiple applications in autumn calculated with v1.2 and with v4.

| Substance | PEC in water V1.2 (µg/L) | PEC in water V4 (µg/L) | Difference (%) | PEC in sediment V1.2 (µg/kg) | PEC in sediment V4 (µg/kg) | Difference (%) |
|-----------|--------------------------------|------------------------------|-------------------|---------------------------------------|-------------------------------------|-------------------|
| 1 | 4.747 | 4.747 | 0.00 | 81.13 | 80.83 | -0.36 |
| 2 | 4.778 | 4.778 | 0.00 | 59.62 | 59.34 | -0.48 |
| 3 | 4.786 | 4.785 | -0.02 | 130.0 | 129.3 | -0.54 |
| 4 | 4.517 | 4.514 | -0.07 | 1600.0 | 1585.6 | -0.90 |
| 5 | 0.04779 | 0.04780 | 0.02 | 0.4800 | 0.4784 | -0.33 |
| 6 | 0.01871 | 0.01870 | -0.05 | 13.75 | 13.70 | -0.36 |

In Table 11 the values for TWAEC21 are compared. The largest difference (6.01%) is found for the substance with a short DegT50 in water, substance 1. For the other substances differences are 1.14% or less, with lower calculated concentrations for v4.

Table 11

TWAEC21 of six parent substances in water and in sediment after multiple applications in autumn calculated with v1.2 and with v4.

| Substance | TWAEC21 in water V1.2 (µg/L) | TWAEC21 in water V4 (µg/L) | Difference (%) |
|-----------|------------------------------------|----------------------------------|-------------------|
| 1 | 0.4495 | 0.4225 | -6.01 |
| 2 | 2.045 | 2.025 | -0.98 |
| 3 | 2.038 | 2.019 | -0.93 |
| 4 | 1.665 | 1.646 | -1.14 |
| 5 | 0.02031 | 0.02010 | -1.03 |
| 6 | 0.004716 | 0.004666 | -1.06 |

Discussion autumn scenario

For the Autumn scenario differences in concentrations calculated by the two versions were less than 2% for all concentrations that were compared, except for the TWAEC21 in water of substance 1 for multiple applications (6.0%). Most concentrations in water calculated with v4 were lower than the concentrations calculated by v1.2. Concentrations in sediment for v4 were higher than v1.2 for the single application, but lower than v1.2 for multiple applications. The relatively large difference in TWAEC21 in water is due to the differences between the models in the way that TWA concentrations are calculated (see discussion Spring scenario).

4 Simulation of metabolites

4.1 Introduction

To calculate exposure concentrations of metabolites with FOCUS_TOXSWA 4.4.3, two options are available:

1. 'Mimicked spray drift entry'; the metabolite is simulated as a spray drift entry. Metabolites are simulated as parent substances. They are mimicked as spray drift events, based on the application rate of the parent corrected for the difference in molar mass and the maximum percentage of metabolite observed in a water-sediment study.
2. 'By degradation'; the formation of the metabolite by degradation of the parent substance is simulated.

The 'mimicked spray drift entry' is currently used with TOXSWA 1.2, and can also be used in FOCUS_TOXSWA 4.4.3. Exposure concentrations of parent substances calculated by FOCUS_TOXSWA 4.4.3 are equal to those calculated by TOXSWA 1.2 (see Chapter 3). Since metabolites are treated in the same way as parent compounds when using the 'mimicked spray drift entry', the model version will not influence the outcome of calculations for metabolites either when using this approach.

FOCUS_TOXSWA 4.4.3 offers the ability to model the formation of metabolites 'by degradation'. The impact of applying this approach instead of the 'mimicked spray drift entry' needs, however, to be investigated. This is described in this chapter. Hence, not the model versions were compared, but the methods to calculate exposure concentrations, by using either calculation procedure in FOCUS TOXSWA 4 and comparing results.

To simulate the fate of metabolites, their properties need to be known. Information on the formation and subsequent degradation of metabolites are often obtained from water-sediment studies. For metabolites, an important parameter is the formation fraction (fraction of the amount of the parent/precursor metabolite that is transformed into the metabolite). When the metabolite is mimicked as a spray drift entry, the maximum percentage of metabolite observed in a water-sediment study is used.

Section 4.2 describes the basic principles of water-sediment studies. Section 4.3 describes the 'mimicked spray drift entry', and Section 4.4 'by degradation', the new procedure in FOCUS_TOXSWA 4.4.3 is described.

To investigate the effect on exposure concentrations of the two approaches of metabolite simulation some calculations were done and presented in Section 4.5.

4.2 Metabolite properties derived from water-sediment study

The conduct of water-sediment studies for pesticides is described in OECD Guideline 308 (OECD, 2002). A short summary of the principles of the study is given, including which results of the studies are currently used to calculate exposure concentrations with TOXSWA for the risk assessment.

Water-sediment systems comprise two interacting compartments (the water column and the sediment layer) subject to different physical, chemical and biological conditions. This can result in quite different degradation behaviour in each of the compartments. Moreover, especially within the sediment there may be large variations in degradation rates between layers of the sediment, due to heterogeneity. E.g., the redox gradient may vary from aerobic conditions at the interface with the water column to strong reduced conditions towards the bottom of the sediment. This affects both the degradation of the parent as well as the formation and degradation of metabolites.

For each of the two options to simulate metabolites parameters derived from the water-sediment study are used. The two options with parameters used are:

1. 'Mimicked spray drift entry'; metabolite is simulated as a spray drift entry.
 - degradation rates of parent and of metabolite in the overall system (water+sediment), and
 - maximum concentration of the metabolite in the overall system.
2. 'By degradation'; the formation of the metabolite by degradation of the parent is simulated.
 - degradation rates of parent and of metabolite in the overall system (water+sediment), and
 - formation fraction of the metabolite in the overall system.

The procedures to determine the parameters from the water-sediment study for these two options are given in the so-called first level (M-I) approach in FOCUS (2006).

4.3 Metabolite simulation using 'mimicked spray drift entry'

In this approach formation of a metabolite in the water body is simulated as a spray drift event, based on the maximum observed percentage of metabolite in the water-sediment study. Therefore the maximum concentration of the metabolite occurs at time zero (i.e. time of the simulated spray drift event). It does not take into account any gradual build-up of the concentration of a metabolite over time. In this approach the simulated maximum concentration of the metabolite can never exceed the observed maximum concentration of the water – sediment study.

The mass entered via spray drift is calculated on the basis of the maximum observed percentage of metabolite in the water-sediment study. The 'drift' loading of the metabolite is calculated using:

$$R_m = R_p \frac{F}{100} \frac{M_m}{M_p} \quad (1)$$

$$L_m = \frac{D}{100} \frac{1}{10} R_m \quad (2)$$

where:

- R_m = metabolite rate of application (kg a.s./ha)
- R_p = parent rate of application (kg a.s./ha)
- 100 = factor for converting % to fraction (-)
- F = maximum observed percentage of formed metabolite (%)
- M_m = molar mass metabolite (g/mol)
- M_p = molar mass parent substance (g/mol)
- L_m = drift loading of metabolite (g/m²)
- 1/10 = factor for converting from kg/ha to g/m² (-)
- D = drift percentage (%)

The 'mimicked spray drift entry' can be applied with TOXSWA 1.2 and with FOCUS_TOXSWA 4.4.3.

4.4 Metabolite simulation using 'by degradation'

In this approach the formation of metabolites in water and in sediment is simulated as a process occurring gradually over time (see Section 1.5, Adriaanse *et al.*, 2014; Beltman *et al.*, 2014). The DegT50 and the formation fraction of the metabolite are needed as input data. In most water – sediment studies the maximum observed percentage is reported and formation fractions are not. It is not appropriate to interpret the maximum observed percentages of metabolites as formation fractions because the maximum observed percentage is the product of both formation and simultaneous degradation. The formation fraction can be estimated from the water-sediment study (FOCUS, 2006). However, it is not always possible to derive reliable formation fractions. In this case, a conservative assumption is that the formation fraction is 1.

The 'by degradation' method can be applied with FOCUS_TOXSWA 4.4.3.

4.5 Impact of using 'by degradation' on exposure calculation

Using the 'by degradation' method instead of the 'mimicked spray drift entry' entails two important differences:

- (1) the increase of metabolite in the system is gradual (rate depending on the DegT50 values of parent and of metabolite) instead of a pulse entry when the metabolite is mimicked as a spray drift entry, and
- (2) the formation fraction is used, instead of the maximum observed percentage of metabolite in the water-sediment study. These are two different entities; the formation fraction is a parameter that can be derived whereas the maximum observed percentage is based on direct observations of specific water-sediment studies.

It is important to note that when a reliable formation fraction cannot be estimated a conservative value for the formation fraction of 1 is applied (see Section 4.4).

In this section the impact of using 'by degradation' is illustrated by some example calculations. The two approaches were compared for the single application scheme with the spring scenario (similar to Chapter 3).

Substance properties

In analogy to the approach in the previous chapter, properties of example metabolites were defined in order to be representative for the range of properties that occur in 'the real world'.

Properties of three metabolites were chosen such that two of the metabolites (M11 and M12) are defined as formation products of substance 1 formed in the water layer, and one metabolite (M21) as formation product of substance 2 formed in the sediment (see Table 12). The substance properties of the parent substances are given in Table 2.

Table 12

Properties of the three example metabolites.

| Substance | Molar mass (g/mol) | Solubility (g/L) | Saturated vapour pressure (Pa) | DegT50 in water at 20 °C (d) | DegT50 in sediment at 20 °C (d) | K_{om} (L/kg) | Freundlich exponent, N (-) |
|-----------|-----------------------|---------------------|-----------------------------------|---------------------------------|------------------------------------|--------------------|---------------------------------|
| M11 | 170 | 0.8 | $1.5 \cdot 10^{-4}$ | 500 | 1000 | 25 | 1 |
| M12 | 140 | 0.8 | $1.5 \cdot 10^{-4}$ | 15 | 1000 | 10 | 1 |
| M21 | 150 | 0.02 | $5 \cdot 10^{-4}$ | 60 | 1000 | 280 | 0.7 |

Input for 'mimicked spray drift entry'

The spray drift loading of the metabolite used in the 'mimicked spray drift entry' is calculated from the maximum observed percentage of the metabolite in the water-sediment study. The maximum observed percentage of the three example metabolites are given in Table 13. Using these percentages, substance properties of parent (Table 2) and of metabolite (Table 12) and application rate (Table 3) with Eqs (1) and (2) results in the spray drift loading mass of metabolite used for the calculations. These are given in Table 14.

Table 13

Maximum observed percentage of the three example metabolites.

| Substance | Parent substance | Max. observed in water (%) | Max. observed in sediment (%) |
|-----------|------------------|-------------------------------|----------------------------------|
| M11 | 1 | 35 | 0 |
| M12 | 1 | 20 | 0 |
| M21 | 2 | 0 | 15 |

Table 14

Spray drift loading (L_m) of metabolite for 'mimicked spray drift entry' based on maximum observed percentage in water-sediment study.

| Substance | Loading spray drift, L_m (mg/m ²) |
|-----------|----------------------------------------------------|
| M11 | 0.198 |
| M12 | 0.090 |
| M21 | 0.093 |

The 'mimicked spray drift entry' simulations are performed with substance properties given in Table 2 and Table 12, the spray drift loadings given in Table 14, and the application schemes given in Table 3. Note that metabolite M21, although formed in sediment, also enters the water layer as a spray drift loading.

Input for 'by degradation'

The simulations are performed with substance properties given in Table 2 and Table 12, the formation fractions given in Table 15, and the application schemes given in Table 3. The formation fractions of the metabolites are not known, and therefore formation fractions of 1 were applied (Table 15).

Table 15

Formation fraction of the three example metabolites.

| Substance | Parent substance | Formation fraction in water (-) | Formation fraction in sediment (-) |
|-----------|------------------|---------------------------------------|------------------------------------------|
| M11 | 1 | 1 | 0 |
| M12 | 1 | 1 | 0 |
| M21 | 2 | 0 | 1 |

Results

The maximum metabolite concentrations in water and in sediment calculated with the two methods are given in Table 16.

Table 16

Metabolite peak concentrations in water and in sediment calculated using 'mimicked spray drift entry' and using 'by degradation'.

| Substance | Parent substance | PEC in water 'mimicked spray drift entry' (µg/L) | PEC in water 'by degradation' (µg/L) | PEC in sediment 'mimicked spray drift entry' (µg/kg) | PEC in sediment 'by degradation' (µg/kg) |
|-----------|------------------|-----------------------------------------------------------|--------------------------------------------|---------------------------------------------------------------|------------------------------------------------|
| M11 | 1 | 0.9427 | 2.545 | 11.81 | 33.58 |
| M12 | 1 | 0.4285 | 2.001 | 3.66 | 18.73 |
| M21 | 2 | 0.4431 | 0.0067 | 24.62 | 4.456 |

The maximum concentrations of the **water metabolites** M11 and M12 in **water** simulated using 'by degradation' are approx. 2.5 times higher (M11) and almost 5 times higher (M12) than the concentrations calculated with the 'mimicked spray drift entry'. These differences are probably due to an overestimation of the formation fraction used in the 'by degradation' method. Formation fractions of 1 were used, because they were not known. The two water metabolites are rapidly formed (DegT50 of parent is 0.2 d⁻¹), which makes the formation of the metabolites nearly similar to the instantaneous input of a drift event, as simulated in the 'mimicked spray drift entry'. This is confirmed by the curves for metabolite M11 shown in Figure 5A. The steep curve of the 'by degradation' method is similar to the vertical curve of the spray drift entry of the 'mimicked spray drift entry'.

The percentages of the PEC value of 'mimicked spray drift entry' to the PEC values of the 'by degradation' method are 37% (M11) and 21% (M12). These values are close to the maximum percentage found in the water-sediment studies used to calculate the spray drift loadings of metabolite in the 'mimicked spray drift entry'. In this special case of a very rapid transformation of the parent, the maximum percentage found in the water-sediment study may very well reflect the formation fractions. For these metabolites formed in water, using formation fractions of 1 with the 'by degradation' method lead to higher exposure concentrations in water in this case. The formation fraction of 1 used for these substances was overestimated.

The maximum concentrations of the **water metabolites** M11 and M12 in **sediment** simulated with the 'by degradation' method are 3 times higher (M11) and 5 times higher (M12) than the concentrations calculated with the 'mimicked spray drift entry'. The higher concentration of the metabolites with 'by degradation' for M11 and M12 can be explained by the higher concentration in water (for M11 see Figure 5A). For these metabolites formed in water, using formation fractions of 1 in the 'by degradation' method leads to higher exposure concentrations in sediment in this case (see also **Figure 5B**). The formation fraction of 1 used for these substances is most likely an overestimation of the unknown true formation fraction.

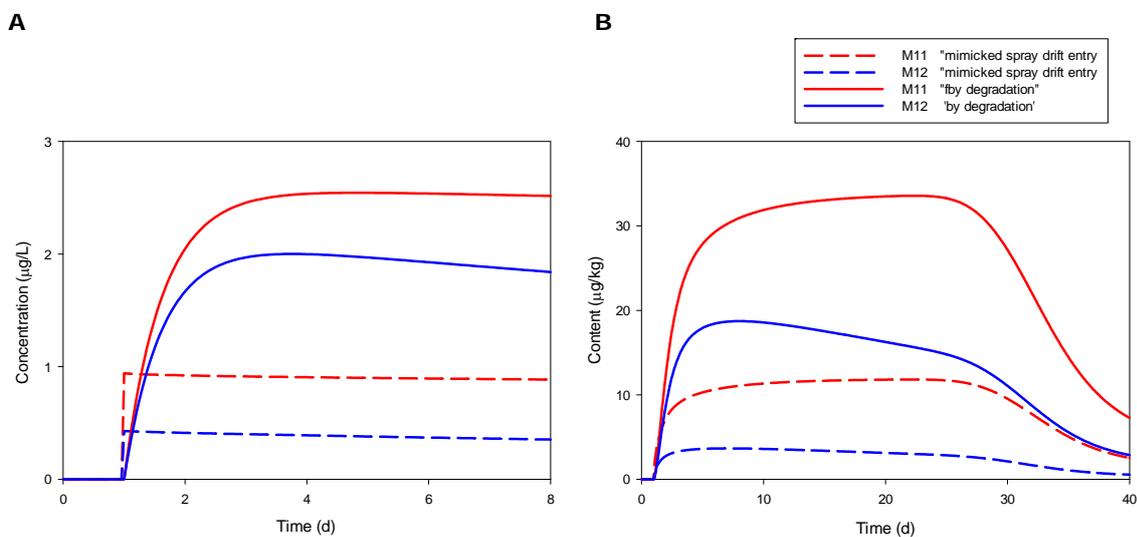


Figure 5 Simulated concentrations of metabolites formed in water by using 'mimicked spray drift entry' by using 'by degradation' (formation fraction = 1), (A) concentration in water, (B) content in sediment.

The maximum concentration of the **sediment metabolite** M21 in **water** calculated using 'by degradation' is almost a factor of 70 lower than with the 'mimicked spray drift entry'. In the 'mimicked spray drift entry' the metabolite M21 enters the water layer directly as a spray drift event. In the 'by degradation' simulation the parent substance must sorb and diffuse from the water layer to the sediment layer, where next the formation of the metabolite M21 occurs; thereafter this metabolite must diffuse back into the water layer. These steps lead to a much lower concentration in water (see **Figure 6A**). For this metabolite formed in sediment using 'by degradation' leads to a much lower exposure concentration in water in this case.

The maximum concentration of the **sediment metabolite** M21 in **sediment** calculated using 'by degradation' is a factor of 10 lower than calculated with the 'mimicked spray drift entry'. In the 'mimicked spray drift entry' the metabolite enters the water layer as a spray drift event, and then sorbs and diffuses into the sediment. In the 'by degradation' simulation the parent must sorb and diffuse from the water layer to the sediment layer, where next the formation of the metabolite M21 occurs. For this metabolite formed in sediment using 'by degradation' leads to a much lower exposure concentration in sediment in this case.

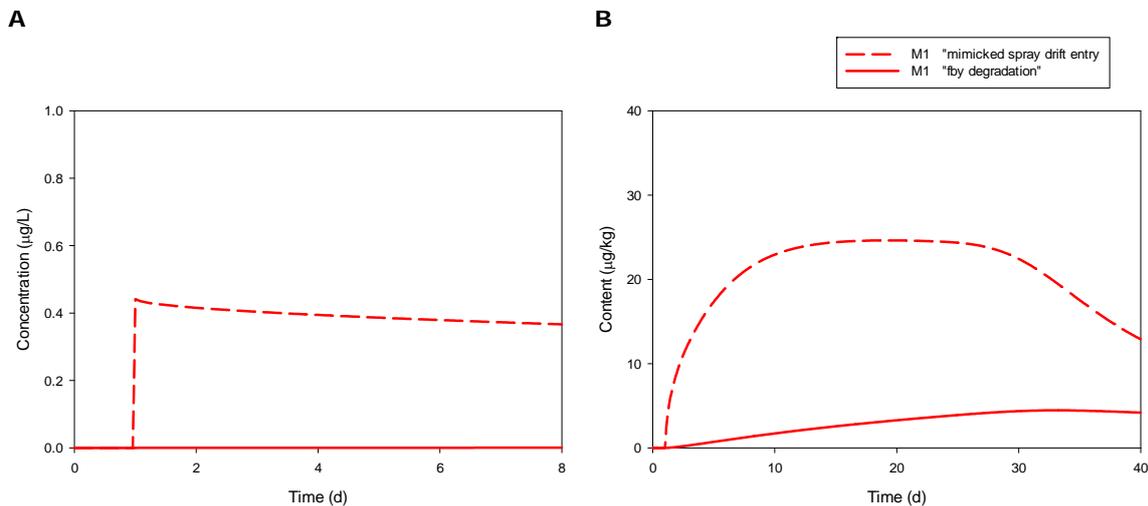


Figure 6 Simulated contents of metabolite formed in sediment with the 'mimicked spray drift entry' and with 'by degradation' (formation fraction = 1) , (A) concentration in water, (B) content in sediment.

Discussion

When metabolites are gradually formed in water or/and in sediment by degradation of the parent, this results in different metabolite concentrations than those resulting from the simulated spray drift deposition.

In the example of the **water metabolites** M11 and M12 in **water** with a very rapid transformation of the parent, the maximum percentage found in the water-sediment study may very well reflect the formation fractions. If the maximum percentage had been used as formation fraction (only possible with rapid transformation) the exposure concentrations would have been equivalent. For metabolites formed in water, using formation fractions of 1 in the 'by degradation' method can lead to higher concentrations in water than with the 'mimicked spray drift entry'. Hence using 'by degradation' may result in higher exposure concentrations in water when the formation fraction of the metabolite is not known, and a worst case formation fraction of 1 is applied. When a known formation fraction is applied using 'by degradation' exposure concentrations can be either lower or higher.

In the example of the **water metabolites** M11 and M12 in **sediment**, the concentrations in sediment simulated using 'by degradation' are higher than the concentrations calculated with the 'mimicked spray drift entry'. The higher concentration of the metabolites using 'by degradation' is explained by the higher concentration in water, due to using a formation fraction of 1 (see above explanation for water metabolites in water). Hence the conclusion given for water metabolites in water is valid for sediment exposure concentrations as well.

In the example of the **sediment metabolite** M21 in **water**, the concentration in water calculated using 'by degradation' was two orders of magnitude lower than with the 'mimicked spray drift entry', because sorption and diffusion to and from sediment delay its appearance in water. Hence, for metabolites formed in sediment using 'by degradation' leads to a lower exposure concentrations in water.

In the example of the **sediment metabolite** M21 in **sediment**, the concentration in sediment calculated using 'by degradation' is one order of magnitude lower than calculated with the 'mimicked spray drift entry'. Hence for metabolites formed in sediment using 'by degradation' leads to a lower exposure concentrations in sediment. When however a parent with a high sorption coefficient degrades fast in the sediment and using a formation fraction of 1, the sediment concentrations could be higher. Therefore, when a known formation fraction is applied using 'by degradation' exposure concentrations can be either lower or higher.

5 Discussion and conclusions

It was investigated whether FOCUS_TOXSWA 4.4.3 can replace TOXSWA 1.2 as the new instrument for simulation of the fate of plant protection products and their metabolites for the NL standard scenarios.

To simulate the NL standard scenarios with FOCUS_TOXSWA 4.4.3 the software available via the FOCUS website, amended with a database and example substances provided via the website www.pesticidemodels.eu can be used. Following a procedure described in this report exposure concentrations can be calculated for spray drift entry of substances. Hence the FOCUS_TOXSWA 4.4.3 software can be used to calculate exposure concentrations for the NL standard scenarios.

For parent substances the differences between the simulated peak concentrations of the two model versions are negligible. The TWAEC21 calculated by TOXSWA 1.2 can be higher than the TWAEC21 calculated by FOCUS_TOXSWA 4.4.3, because TOXSWA 1.2 interpolates intermediate daily concentrations linearly, ignoring the exponential decrease (see Section 3.3). TOXSWA v1.2 overestimates the TWAEC values, where the overestimation is highest for substances with very short half-lives (approx. 5% for DegT50 of 0.2 d).

It can be concluded that the match between the two model versions is satisfactory and as expected for parent substances. Exposure concentrations for parent substances calculated with FOCUS_TOXSWA 4.4.3 are the same as those calculated by TOXSWA 1.2, and TWAEC values calculated by FOCUS_TOXSWA 4.4.3 are more accurate.

For metabolite substances, there are differences in simulation results between the two model versions. These differences were anticipated and are the consequence of the different methods used to calculate metabolite formation. TOXSWA 1.2 does not simulate metabolite formation. The metabolite formation is mimicked as a spray drift event ('mimicked spray drift entry'), with an application rate based on the application rate of the parent corrected for the difference in molar mass and the maximum percentage of metabolite observed in a water-sediment study. This can also be done with FOCUS_TOXSWA 4.4.3. FOCUS_TOXSWA 4.4.3 simulates metabolite formation from the parent, using the formation fraction of the metabolite fitted from a water-sediment study or the maximal formation fraction of 1 when it is not known. Results with the new model (FOCUS_TOXSWA 4.4.3) are considered a better estimate of the actual exposure because of increased conceptual soundness of the model.

When FOCUS_TOXSWA 4.4.3 is used for metabolites and its functionality 'by degradation' is used, the effect on calculated exposure concentrations as compared to the 'mimicked spray drift entry' based on the example calculations done in this study are:

- **metabolites formed in water;** higher exposure concentrations in water and in sediment when the formation fraction of the metabolite is not known, and a worst case formation fraction of 1 is applied. When a known formation fraction is applied exposure concentrations can be either lower or higher.
- **metabolites formed in sediment;** lower exposure concentrations in water and also lower exposure concentration in sediment.

When a known formation fraction is applied exposure concentrations can be either lower or higher.

When the formation fraction of the metabolite is not known there are two options for simulation of metabolites with FOCUS_TOXSWA 4.4.3: (i) use a formation fraction of 1, or (ii) use the maximal fraction observed in the water-sediment study and mimic the metabolite as a spray drift event (i.e. same approach as for TOXSWA 1.2).

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- FOCUS (2006). *Guidance Document on Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration*. Report of the FOCUS Work Group on Degradation Kinetics, EC Document Reference Sanco/10058/2005 version 2.0, 434 pp.
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<http://dx.doi.org/10.1787/9789264070523-en>.
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Justification

Since 1999 TOXSWA 1.2 is used in the authorization procedure of plant protection products in the Netherlands. TOXSWA calculates exposure concentrations for aquatic organisms for two NL standard scenarios (Beltman and Adriaanse, 1999b). The use of TOXSWA 1.2 is described in a manual (Beltman and Adriaanse, 1999a). The current report describes how the software used now (TOXSWA 1.2) can be replaced by FOCUS_TOXSWA 4.4.3 to calculate exposure concentrations for the two NL standard scenarios.

The content of this report was reviewed by John Deneer of Wageningen Environmental Research (Alterra). The project was supervised by Jennie van der Kolk (contact Statutory Research Unit for Nature and the Environment (WOT Natuur & Milieu)), theme Agri-Environment) and seen and approved by Anja van Gernerden (Ministry of Economic Affairs).

Annex 1 Example of FOCUS_TOXSWA version 4 input file

This annex shows an example of the txw input file of FOCUS_TOXSWA 4.4.3 for the NL spring scenario.

The TOXSWA input file of a TOXSWA run with the NL drift Spring scenario and substance EXNL1.

```
**-----
* TOXSWA input file
* INPUT FILE for TOXSWA 3 version (f90)
*-----
* This file is intended to be used by expert users.
*
* Contact address:
* -----
* Wim Beltman
* Alterra
* PO BOX 47
* 6700 AA Wageningen
* The Netherlands
* e-mail: wim.beltman@wur.nl
*
* (c) Alterra
*
*-----
*
* Section 1: Control Section
*-----
*
01-Oct-1985      TimStart      ! Start date of simulation [01-Jan-1900 - 31-Dec-9999]
30-Oct-1985      TimEnd        ! End date of simulation [01-Jan-1900 - 31-Dec-9999]
FOCUS           CallingProgram ! Calling program in FOCUS_TOXSWA for EU authorization
4               CallingProgramVersion ! Version of calling program
4               ModelVersion    ! version number of the model
4               GUIVersion      ! version number of the GUI
2               DBVersion       ! version number of the database
Hourly          OptInp          ! Option for hourly or daily input data (Hourly, Daily)
OnLine         OptHyd          ! Hydrology simulation option (Only, OnLine, OffLine,
Automatic)
OnLine         OptTem          ! Temperature simulation option (Only, OnLine, OffLine,
Automatic)
600            MaxTimStpWat (s) ! Maximum calculation time step in water layer [0.001 - 3600]
600            MaxTimStpSed (s) ! Maximum calculation time step in sediment [0.001 - 3600]
600.           TimStpHyd (s)   ! Maximum calculation time step for hydrology [0.001 - 3600]
No             OptScreen       ! Option to show output on screen (Yes, No)
Calc          OptTimStp       ! Time step substance simulation options (Input, Calc)

*-----
*
* Section 2: Waterbody section
*-----
*
NL_spring      Location        ! Name of the location
NL_spring      WaterbodyID     ! ID of the water body

* Table WaterBody
* Len          = Length (m) [0.1 - 10000]
* NumSeg       = Number of segments (-) [1 - 1000]
* WidWatSys    = Width of the bottom of water system (m) [0.1 - 100]
* SloSidWatSys = Side slope of the water system (-) [0.001 - 2]
* DepWatDefPer = Water depth defining perimeter for the exchange between water layer and sediment (m)
[0 - lowest water depth]

table WaterBody
Len          NumSeg    WidWatSys SloSidWatSys DepWatDefPer
(m)          (-)       (m)       (-)           (m)
320.         80        0.4       1.             0.1
End_table

15.          ConSus (g.m-3)      ! Concentration of suspended solids [1.0 - 100000]
0.5         CntOmSusSol (kg.kg-1) ! Mass ratio of organic matter in suspended solids [0.0
- 1.0]
0.          AmaMphWatLay (g.m-2) ! Dry weight of macrophyte biomass per m2 bottom [0.0 -
1000]
```

```

*-----
*
* Section 3: Hydrology: general
*-----
*
Constant          OptWaterSystemType ! Option for selecting the water system type (Pond,
WaterCourse)
Constant          OptFloWat          ! Option for water flow (Constant, Variable)

* if: OptWaterSystemType = WaterCourse
Input             OptDis             ! Options are 'Fischer' and 'Input'

* if: OptDis = Input
20.               CofDisPhsInp (m2.d-1) ! Dispersion coefficient [0. - 100000]
*-----
*
* Section 3a: Constant water flow
*-----
*
* if: OptFloWat = Constant
0.3               DepWat (m)
10.               VelWatFlwBas (m.d-1)
*-----
*
* Section 3b: Variable water flow: pond
*-----
*
* if: OptFloWat = Variable and OptWaterSystemType = Pond
0.45              AreaSurPndInp (ha)    ! Size of area surrounding the pond [0.0 - 50.0]

* if: CallingProgram = FOCUS
2.193            QBasPndInp (m3.d-1)    ! Base flow, i.e. inflow into pond [0.001 - 50.0]
1.               HgtCrePnd (m)         ! Height of the weir crest [0.1 - 5.0]
0.5              WidCrePnd (m)         ! Width of the weir crest [0.01 - 10]

* if: Opt = Runoff
0.06             AreaErsSurPndInp (ha) ! Size of the eroding area around the pond [0.0 - 50.0]
*-----
*
* Section 3c: Variable water flow: watercourse
*-----
*
* if: OptFloWat = Variable and OptWaterSystemType = WaterCourse
*representative channel
0.0001           SloBotRepCha (-)      ! Slope bottom representative channel [0.0 - 0.01]
0.4              HgtCreRepCha (m)      ! Height of the weir crest [0.1 - 5.0]
0.5              WidCreRepCha (m)      ! Width of the weir crest [0.01 - 10]

1000.            LenRepCha (m)         ! Length representative channel [10.0 - 2000]
1.               WidBotRepCha (m)      ! Width bottom representative channel [0.1 - 10]
1E-005           SloSidRepCha (-)      ! Side slope of the representative channel [0.0 - 10]

25.              CofRghRef (-)         ! Value of the Manning coefficient for bottom roughness [1.0 -
100]
1.2             CofVelHea (-)         ! Energy coefficient resulting from the non-uniform distribution
of flow velocities [1.1 - 1.5]

* if: CallingProgram = NL or FOCUS
2.               AreaUpsWatCrSInp (ha) ! Size of the area upstream the representative channel
[0.0 - 10000]
0.66            QBasWatCrSInp (m3.d-1) ! Minimal flow into watercourse [0.0 10000]

2.               AreaUpStrRepCha (ha)  ! Size of the area upstream the representative channel
[0.0 - 10000]
1.               QBasRepCha (m3.d-1)   ! Minimal flow into watercourse [0.0 - 10000]
*-----
*
* Section 4: Sediment section
*-----
*
NL_drift          SedimentTypeID      ! Name of sediment type

* table SedimentProfile
* ThiHor = thickness of horizon [0.0001 - ]
* NumLay = number of layers in horizon [1,]

table SedimentProfile
ThiHor    NumLay
(m)
0.004     4
0.006     3
0.01      2
0.02      2
0.06      4
end_table

```

```

Input                OptSedProperties  ! Option sediment properties [Input, Calc]

* table specifying SedimentProperties for each horizon:
* Nr                = number horizon [1,]
* Rho               = bulk density [100 - 2000]
* CntOm             = organic matter mass content [0.1 - 1.0]
* ThetaSat         = saturated water content [0.1 - 0.95]
* CofDifRel        = relative diffusion coefficient [0.0 - 1.0]

table horizon SedimentProperties
Nr      Rho      CntOm      ThetaSat  CofDifRel
      (kg.m-3) (kg.kg-1) (m3.m-3) (-)
1       80.     0.25     0.82     0.82
2       80.     0.25     0.82     0.82
3      220.     0.19     0.77     0.77
4      670.     0.06     0.77     0.77
5     1500.     0.02     0.36     0.28
end_table

0.                FlwWatSpg (m3.m-2.d-1)

* If: FlwWatSpg not zero
* table horizon DispersionLength
* Nr                = Horizon number []
* LenDisSedLiq     = Dispersion length of solute in liquid phase [0.05 - 1.0]

table horizon DispersionLength
Nr      LenDisSedLiq
      (m)
1       0.015
2       0.015
3       0.015
4       0.015
5       0.015
end_table

* If: OptLoa = PRZM
0.01      ThiLayErs (m)      ! Thickness of sediment layer to which eroded soil is added
[0.0001 - ]
*-----
*
* Section 5: Weather section
*-----
*

NL_drift      MeteoStation  ! Name of the *.met file with meteo data

Monthly      OptMetInp     ! Option for hourly or daily input data (Hourly, Daily, Monthly)

*-----
*
* Section 6: Compound section
*-----
*

EXNL1      SubstanceName  ! Name of parent substance [1 - 6 characters]

table compounds      ! List of substances [1 - 6 characters]
EXNL1
end_table

* Table parent-daughter relationships transformation in water (FraPrtDauWat):
* Column 1: fraction formed from parent into daughter
* Column 2: name of parent
* Column 3: name of daughter

table FraPrtDauWat (mol.mol-1)
end_table

* Table parent-daughter relationships transformation in sediment (FraPrtDauSed):
* Column 1: fraction formed from parent into daughter
* Column 2: name of parent
* Column 3: name of daughter

Table FraPrtDauSed (mol.mol-1)
end_table

* Substance properties for each substance given in table compounds
* Substance code is extension of parameter name
*----- Parent: EXNL1 -----

350.6      MolMas_EXNL1 (g.mol-1)  ! Molar mass of parent substance [10.0 - 10000]

75.3      DT50WatRef_EXNL1 (d)    ! Half-life transformation in water [0.1 - 100000]
20.      TemRefTraWat_EXNL1 (C)  ! Temperature at which half-life was measured [5.0 - 30]
55.      MolEntTraWat_EXNL1 (kJ.mol-1) ! Molar activation enthalpy of transformation in
water [0.0 - 200]

```

```

100.          DT50SedRef_EXNL1 (d)  ! Half-life transformation in sediment [0.1 - 100000]
20.          TemRefTraSed_EXNL1 (C) ! Temperature at which half-life was measured [5.0 - 30]
55.          MolEntTraSed_EXNL1 (kJ.mol-1) ! Molar activation enthalpy of transformation in
sediment [0.0 - 200]

16400.       KomSed_EXNL1 (L.kg-1)  ! Coefficient of equilibrium sorption in sediment [0.0 -
100000000]
0.001       ConLiqRefSed_EXNL1 (mg.L-1) ! Reference concentration in liquid phase in
sediment [0.001 - 100]
0.9         ExpFreSed_EXNL1 (-)     ! Freundlich exponent in sediment [0.1 - 2]
16400.       KomSusSol_EXNL1 (L.kg-1) ! Coefficient of equilibrium sorption suspended
solids [0.0 - 10000000]
0.001       ConLiqRefSusSol_EXNL1 (mg.L-1) ! Reference concentration in liquid phase
suspended solids [0.001 - 100]
0.9         ExpFreSusSol_EXNL1 (-) ! Freundlich exponent suspended solids [0.1 - 2]

0.          CofSorMph_EXNL1 (L.kg-1) ! Coefficient for linear sorption on macrophytes [0.0
- 20000]

0.0025      PreVapRef_EXNL1 (Pa) ! Saturated vapour pressure [0.0 - 200000]
20.         TemRefVap_EXNL1 (C) ! Temperature of reference at which the saturated vapour
pressure was measured [0.0 - 40]
95.         MolEntVap_EXNL1 (kJ.mol-1) ! Molar enthalpy of the vaporization process [-200 -
200]

2.          SlbWatRef_EXNL1 (mg.L-1) ! Water solubility [0.001 - 1000000]
20.         TemRefSlb_EXNL1 (C) ! Temperature of reference at which the water solubility
was measured [0.0 - 40]
27.         MolEntSlb_EXNL1 (kJ.mol-1) ! Molar enthalpy of the dissolution [-200 - 200]
4.E-5       CofDifWatRef_EXNL1 (m2.d-1) ! Reference diffusion coefficient in water [0.0 -
200]

*-----
*
* Section 7: Management section
*-----
*
* Loading options (OptLoa):
* DriftOnly = spray drift only entry route
* PEARL     = drainage calculated by PEARL
* MACRO     = drainage calculated by MACRO
* PRZM      = runoff and erosion calculated by PRZM
* GEM       = point source calculated by GEM

DriftOnly      OptLoa          ! Loading options (DriftOnly, PEARL, MACRO, PRZM, GEM)

FOCUS_EXAMPLE ApplicationScheme ! Name of the application scheme

* Table loadings
* Column 1: Date of application, relevant if OptLoa = DriftOnly, otherwise the date is a dummy values
* Column 2: Type of loading (-)
* Column 3: Drift deposition (mg.m-2) []
* Column 4: Start of stretch of watercourse loaded by all loading types (m) []
* Column 5: End of stretch of watercourse loaded by all loading types (m)[]

table Loadings
10-Oct-1985  drift      1.          20.          320.
end_table

* If: OptLoa = MACRO or OptLoa = PRZM
* Table with path+name of lateral entries files

table Soil substance files
end_table

* If: OptLoa = PEARL or OptLoa = MACRO
100.         WidFldDra (m)          ! Width of field contributing drainage

* If: OptLoa = PRZM
100.         WidFldRnf (m)          ! Width of field contributing runoff
20.         WidFldErs (m)          ! Width of field contributing erosion
0.          RatInfDir (-)          ! Ratio of infiltration water added to runoff water

* If: CallingProgram = FOCUS and OptWaterSystemType = WaterCourse
Yes          OptUpsInp             ! Switch for upstream catchment treated (Yes, No)
0.          RatAreaUpsApp (-)      ! Ratio of upstream catchment treated [0.0 - 1]
1.          FraMetForUps (-)      ! Fraction primary metabolites formed in water in upstream
catchment
0.          ConAir (kg.m-3)        ! Concentration of the substance in air
0.          ConWatSpq (g.m-3)      ! Concentration in incoming seepage water

0.          ConSysWatIni (g.m-3)

* Table initial substance content in sediment (CntSysSedIni)
* Column 1: Depth in sediment (m)
* Column 2: Substance content (mg.kg-1)
table interpolate CntSysSedIni (mg.kg-1)
end_table
*-----
*

```

```

* Section 8: Output control
*-----
*
No          OptDelOutFiles  ! Switch for removing *.out files after run (Yes, No)
FOCUS      OptReport       ! Options for report type (DutchRegistration, FOCUS)
Yes        ExposureReport ! Exposure report (Yes, No)
No         PercentileReport ! Percentile report (Yes, No)
DaysFromSta DateFormat    ! Date format (DaysFromSta, DaysFrom1900, Years)
e14.6      RealFormat     ! Number format of the reals

0.01       ThiLayTgt (m)   ! Thickness of the target layer
Hour       OptDelTimPrn  ! Option to set output time step (Hour, Day, Decade, Month, Year,
Automatic, Other)
1          DelTimPrn (d)   ! Output time step [0.0 - length simulation period]
No         PrintCumulatives ! Specify whether fluxes should be cumulated over the entire simulation
period (Yes, No)

* table HorizontalProfiles: dates are given for which detailed output is wished
* Column 1: dates

table HorizontalProfiles
end_table

* Table output depths (OutputDepths): indicate for which depths the output is selected
* Column 1: Depth

table OutputDepths (m)
end_table

All OptOutputDistances ! Switch output distances (None, All, Table)

* Table output distances (OutputDistances): indicate for which distance the output is selected
* Column 1: Distance

table OutputDistances (m)
end_table

No          print_VelWatFlw    ! Flow velocity (m/h) [Yes, No]
No          print_QBou       ! Discharge (m3/h) [Yes, No]
No          print_VvrLiqDra   ! Drain flow (m/h) [Yes, No]
No          print_VvrLiqRnf   ! Runoff flow [Yes, No]
No          print_FlmDra      ! Drain substance flux [Yes, No]
No          print_FlmRnf      ! Runoff substance flux [Yes, No]
No          print_FlmErs      ! Erosion substance flux [Yes, No]
Yes         print_ConLiqWatLay ! Concentration in water, hour average (g/m3) [Yes, No]
No          print_ConSysWatLay ! Total concentration in water (g/m3) [Yes, No]
No          print_CntSorMph    ! Content sorbed to macrophytes [Yes, No]
No          print_CntSorSusSol ! Content sorbed suspended solids [Yes, No]
No          print_ConSysSed    ! Total content in sediment [Yes, No]
No          print_ConLiqSed    ! Concentration in pore water sediment (g/m3) [Yes, No]
No          print_CntSorSed    ! Content sorbed to sediment [Yes, No]
No          print_DepWat       ! Water depth (m) [Yes, No]
No          print_DepWatRepCha ! Water depth representative channel [Yes, No]
Yes         print_CntSedTgt    ! Total content in target layer sediment [Yes, No]
No          print_ConLiqSedTgt ! Concentration in pore water in target layer sediment [Yes, No]
No          print_CntSorSedTgt ! Content sorbed in target layer sediment [Yes, No]
Yes         print_ConLiqWatLayCur ! Concentration in water, at end hour (g/m3) [Yes, No]
Yes         print_AmaWatLay    ! Mass in water layer [Yes, No]
Yes         print_AmaLiqWatLay ! Mass in liquid phase in water layer [Yes, No]
Yes         print_AmaSorSusSol ! Mass sorbed to suspended solids in water layer [Yes, No]
Yes         print_AmaSorMph    ! Mass sorbed to macrophytes in water layer [Yes, No]
Yes         print_AmaSed       ! Mass in sediment layer [Yes, No]
Yes         print_AmaLiqSed    ! Mass in liquid phase in sediment layer [Yes, No]
Yes         print_AmaSorSed    ! Mass sorbed in sediment layer [Yes, No]
Yes         print_AmaTraWatLay ! Mass transformed in water layer [Yes, No]
Yes         print_AmaForWatLay ! Mass formed in water layer [Yes, No]
Yes         print_AmaVolWatLay ! Mass volatilised in water layer [Yes, No]
Yes         print_AmaSedInWatLay ! Mass penetrated into sediment from water layer [Yes, No]
Yes         print_AmaSedOutWatLay ! Mass transferred from sediment into water layer [Yes, No]
Yes         print_AmaDwnWatLay ! Mass flowed across downstream boundary out of water layer [Yes,
No]
Yes         print_AmaUpsWatLay ! Mass flowed across upstream boundary into water layer [Yes,
No]
Yes         print_AmaDrfWatLay ! Mass entered water layer by spray drift [Yes, No]
Yes         print_AmaAtmDepWatLay ! Mass entered water layer by atmospheric deposition [Yes, No]
Yes         print_AmaDraWatLay ! Mass entered water layer by drainage [Yes, No]
Yes         print_AmaRnoWatLay ! Mass entered water layer by runoff [Yes, No]
Yes         print_AmaTraSed    ! Mass transformed in sediment layer [Yes, No]
Yes         print_AmaForSed    ! Mass formed in sediment layer [Yes, No]
Yes         print_AmaWatLayInSed ! Mass transferred into water layer from sediment layer [Yes,
No]
Yes         print_AmaWatLayOutSed ! Mass transferred from water layer into sediment layer [Yes,
No]
Yes         print_AmaDwnSed    ! Mass leaving sediment layer across lower boundary [Yes, No]
Yes         print_AmaErsSed    ! Mass entering sediment layer by erosion [Yes, No]
No          print_VolErrWatLay ! Volume error in waterbody [Yes, No]
No          print_AmaErrWatLay ! Mass error in mass balance of the waterlayer [Yes, No]
No          print_ConLiqWatLayNLAvg ! Concentration in water, average in evaluation stretch [Yes,
No]

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* End of TOXSWA input file
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